

On paths, stars and wyes in trees

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Abstract

We further the study of local profiles of trees. Bubeck and Linial showed that the set of 5-profiles contains a certain polytope, namely the convex hull of d -millipedes, and they proved that the segment [0-millipede, 1-millipede] corresponds to a face of the set of 5-profiles. Our main result shows that the segment [1-millipede, 2-millipede] also corresponds to a face. Surprisingly we also show that for $d \geq 4$ the segment [d -millipede, $(d+1)$ -millipede] is not a face of the set of 5-profiles. We do so by exhibiting new trees which are generalized millipedes with intriguing patterns for their degree sequence. The plot thickens, and the set of 5-profiles remains a mysterious convex set.

1 Introduction

We study the notion of local profiles of trees introduced by Bubeck and Linial in [1] (henceforth BL). We focus mostly on 5-profiles: for a tree T let $P(T)$ be the number of 5-vertex paths in T , $S(T)$ the number of 5-vertex stars in T , and $Y(T)$ the number of 5-vertex “wyes” in T . We simply write S, P and Y when T is clear from the context. BL proved that all trees satisfy the following linear relation between those quantities: $Y \leq 36S + P + 4$. Our main contribution is to prove a tighter bound that was suggested in [Open problem 1, BL].

Theorem 1 *All trees satisfy*

$$Y \leq 9S + P + 6.$$

This bound is optimal in the sense that for any $M \in \mathbb{N}$ there exists a tree T with $P, S, Y \geq M$ and $Y = 9S + P$ (see [Section 5, BL]). In particular as explained in [Open problem 1, BL] this new bound characterizes one of the face of the set of 5-profiles $\Delta_{\mathcal{T}}(5)$ (see below for a precise definition of the set of k -profiles $\Delta_{\mathcal{T}}(k)$) which corresponds to the convex hull of 1-millipede and 2-millipede. Yet, perhaps surprisingly, we exhibit in Section 3 new trees whose 5-profiles are outside the convex hull of simple millipedes (thus proving that [(9), BL] is a strict inclusion and completing the answer to [Open Problem 1, BL]).

We also answer positively [Open problem 3, BL] (a similar result was recently and independently obtained in [2]): we prove that if the proportion of k -vertex paths among k -vertex subtrees (denoted p_1 , see below for the more precise definition) goes to zero, then the proportion of k -vertex stars (denoted p_2) goes to 1. In fact our explicit bound given below also gives a partial answer to [Open problem 7, BL] as it is a non-linear relation between p_1 and p_2 .

Theorem 2 *Let $k \geq 6$ and $p \in \Delta_{\mathcal{T}}(k)$, then*

$$p_2 \geq 1 - e(k-1)!(k-1)^{\frac{1-\varepsilon}{k-1}}, \text{ where } \varepsilon = \frac{k-2 + \sqrt{(k-2)^2 + 4(k-2)}}{2}.$$

If $p \in \Delta_{\mathcal{T}}(5)$, then

$$p_2 \geq 1 - p_1 - 2 \cdot 4^{2+\sqrt{3}} p_1^{\frac{2-\sqrt{3}}{4}}.$$

For sake of convenience for the reader we recall the precise definition of k -profiles. For (unlabelled) trees T, R , we denote by $c(R, T)$ the number of copies of R in T , or in other words the number of injective homomorphism from R to T . Let $T_1^k, \dots, T_{N_k}^k$ be a list of all isomorphism types of k -vertex trees. The k -profile of a tree T is the vector $p^{(k)}(T) \in \mathbb{R}^{N_k}$ whose i -th coordinate is

$$(p^{(k)}(T))_i = \frac{c(T_i^k, T)}{Z_k(T)}, \text{ where } Z_k(T) = \sum_{j=1}^{N_k} c(T_j^k, T).$$

We focus on the set of k -profiles attainable with large trees:

$$\Delta_{\mathcal{T}}(k) = \left\{ p \in \mathbb{R}^{N_k} : \exists (T_n), |T_n| \xrightarrow{n \rightarrow \infty} \infty, \text{ and } p^{(k)}(T_n) \xrightarrow{n \rightarrow \infty} p \right\},$$

where $|T|$ denotes the number of vertices in T . In the rest of the paper $D(T)$ denotes the largest degree in T , and $d_T(v)$ denotes the degree of vertex v in T (when the tree is clear from the context we drop the reference to T).

2 Proof of Theorem 1

Our approach is quite different from BL's proof of the weaker bound $Y \leq 36S + P + 4$. In particular we use simple inductive arguments which avoid the pedestrian counting that BL used to rewrite $P - Y$ as a linear combination of the number of vertices of certain "types". On the other hand the inductive step in the BL proof relied on a special way of cutting a tree, and our proof is centered around an extension of such cuts. Precisely for $i, j \in \mathbb{N}$ we define the (i, j) -cut of a tree T around (u, v) (where $\{u, v\}$ is an edge) as follows: remove the edge $\{u, v\}$, and add a path of length i to u and a path of length j to v . When u, v, i , and j are clear from the context, we denote T_1 and T_2 the two trees in the forest obtained after the (i, j) -cut, such that $u \in T_1$ and $v \in T_2$. The BL proof used only $(1, 0)$ -cuts, while we use $(0, 0)$, $(1, 0)$, $(1, 1)$ and $(2, 1)$ -cuts.

The proof of Theorem 1 proceeds in two steps: first we prove it for trees such that $D \leq 4$, and then we extend it to the general case. This is similar to what BL did, as they first proved $Y \leq 36S + P + 4$ when $D \leq 3$ (in which case it rewrites $Y \leq P + 4$) and then extended to the general case.

We start with a simple lemma which shows that, without loss of generality, we can focus on trees without degree 2 vertices.

Lemma 1 *If there exists a tree such $Y > 9S + P + 6$, then there exists a tree without degree 2 vertices which also satisfy this inequality.*

Proof Assuming that there exists trees with $Y > 9S + P + 6$, let T be the smallest such tree. We will now show by contradiction that T cannot have degree 2 vertices. Let us assume that it does. Then there exist vertices v and w , each with degree at least 3 that are joined by a path P of length at least 2, all of whose internal vertices have degree 2. Let the tree T' be obtained from T by replacing P with a single edge vw . Clearly $S(T') = S(T)$. We also have

$$Y(T') = Y(T) + \binom{d(v)-1}{2}(d(w)-2) + \binom{d(w)-1}{2}(d(v)-2)$$

and

$$P(T') \leq P(T) + \sum_{\substack{x \sim v \\ x \notin V(P)}} (d(x)-1)(d(w)-2) + \sum_{\substack{x \sim w \\ x \notin V(P)}} (d(x)-1)(d(v)-2).$$

By the minimality of T we have $Y(T') \leq 9S(T') + P(T') + 6$, and so $P(T') - P(T) > Y(T') - Y(T)$. In particular we may assume that

$$\sum_{\substack{x \sim w \\ x \notin V(P)}} (d(x)-1) > \binom{d(w)-1}{2}. \quad (1)$$

We now consider two cases:

Case 1: $d(v) \geq 4$ or $d(w) \geq 4$.

We consider the $(2, 1)$ -cut around (v, w) . Observe first that $S(T) = S(T_1) + S(T_2)$. Now

$$Y(T) - Y(T_1) - Y(T_2) = \binom{d(w) - 1}{2}.$$

Further

$$P(T) - P(T_1) - P(T_2) \geq (d(v) - 1) + (d(w) - 1) + \sum_{\substack{x \sim w \\ x \notin V(P)}} (d(x) - 1).$$

Therefore

$$\begin{aligned} Y(T) &\leq Y(T_1) + Y(T_2) + \binom{d(w) - 1}{2} \\ &\leq 9S(T) + P(T) + 12 + \binom{d(w) - 1}{2} - (d(v) - 1) - (d(w) - 1) - \sum_{\substack{x \sim w \\ x \notin V(P)}} (d(x) - 1). \end{aligned}$$

The lemma follows from (1).

Case 2: $d(v) = d(w) = 3$.

We consider the $(1, 1)$ -cut around (v, w) . Again $S(T) = S(T_1) + S(T_2)$. Now we have

$$Y(T) - Y(T_1) - Y(T_2) = 2$$

and

$$\begin{aligned} P(T) - P(T_1) - P(T_2) &\geq (d(v) - 1) + (d(w) - 1) + \sum_{\substack{x \sim v \\ x \notin V(P)}} (d(x) - 1) + \sum_{\substack{x \sim w \\ x \notin V(P)}} (d(x) - 1) \\ &\geq 6 + \sum_{\substack{x \sim v \\ x \notin V(P)}} (d(x) - 1), \end{aligned}$$

where the last inequality used (1). Now observe that if

$$\sum_{\substack{x \sim v \\ x \notin V(P)}} (d(x) - 1) \geq 2, \text{ or } \sum_{\substack{x \sim v \\ x \notin V(P)}} (d(x) - 1) = 0,$$

then we are done. On the other other hand if this sum is equal to 1, then v is adjacent to two vertices of degree 2 and one leaf x . But then consider $T'' = T \setminus x$. We have $Y(T'') = Y(T) - 2$ and $P(T'') \leq P(T) - 2$, contradicting the minimality of T . This completes the proof of the lemma. ■

Proposition 1 *If $D \leq 4$, then $Y \leq 9S + P + 6$.*

Proof We say that a 5-vertex subtree S of T is centered at $v \in V(T)$ if $v \in V(S)$ and S is a star and v has degree 4 in S ; if S is a path and v is the middle vertex; or if S is a wye and v has degree 3 in S . For each vertex $v \in V(T)$ denote by $S(v)$, $P(v)$ and $Y(v)$ the number stars, paths and wyes, resp., centred at v . Let us also define $\gamma(v) = 2 - d'(v)$, where $d'(v)$ denotes the number of non-leaf neighbours of v . Observe that $\sum_v \text{non-leaf } \gamma(v) = 2$. Thus is enough to show that $9S(v) + P(v) - Y(v) + 3\gamma(v) \geq 0$ for any non leaf-vertex v . Recall also the formulas

$$S(v) = \binom{d(v)}{4}$$

and

$$P(v) = \sum_{u, w \sim v} (d(u) - 1)(d(w) - 1)$$

and

$$Y(v) = \sum_{u \sim v} (d(u) - 1) \binom{d(v) - 1}{3}.$$

We now consider two cases:

Case 1: $d(v) = 4$.

It suffices to verify that for each $k \leq 4$ and every choice of $x_1, \dots, x_k \in \{2, 3\}$ we have

$$\sum_{i=1}^k 3(x_i + 1) - 1 \leq 15 + \sum_{1 \leq i < j \leq k} x_i x_j,$$

which is indeed true.

Case 2: $d(v) = 3$.

It suffices to verify that for each $k \leq 3$ and every choice of $x_1, \dots, x_k \in \{2, 3\}$ we have

$$\sum_{i=1}^k (x_i + 3) - 1 \leq 6 + \sum_{1 \leq i < j \leq k} x_i x_j.$$

which is again true. ■

We can now move to the proof of Theorem 1.

Proof We prove the inequality by induction. Let u be a vertex of maximal degree in T , such that at most one of its neighbors has degree $D(T)$ (clearly such a vertex exist). Let v be a neighbor of u of maximal degree. Denote $a = d(v)$ and $d = D(T)$. We will either consider the $(0, 0)$ -cut or the $(0, 1)$ -cut of T around (u, v) , and then apply the induction hypothesis on T_1 and T_2 , i.e., $Y(T_i) \leq 9S(T_i) + P(T_i) + 6$. Thus we have to show that the number of paths removed (denoted δ_P), plus nine times the number of stars removed (denoted δ_S), is at least six plus the number of wyes removed (denoted δ_Y).

In the case of a $(0, 0)$ -cut one has:

$$\begin{aligned} \delta_S &= 9 \binom{d}{4} - 9 \binom{d-1}{4} + 9 \binom{a}{4} - 9 \binom{a-1}{4} \\ &= \frac{3}{2} (d-1)(d-2)(d-3) + \frac{3}{2} (a-1)(a-2)(a-3), \end{aligned}$$

and

$$\delta_P \geq (a-1) \sum_{\substack{w \sim u \\ w \neq v}} (d(w) - 1) + (d-1) \sum_{\substack{w \sim v \\ w \neq u}} (d(w) - 1),$$

and

$$\begin{aligned} \delta_Y &= \binom{a-1}{2} (d-1) + \binom{d-1}{2} (a-1) + \\ &\quad + \sum_{\substack{w \sim u \\ w \neq v}} \binom{d(w)-1}{2} + (d-2) \left(\sum_{\substack{w \sim u \\ w \neq v}} d(w) - 1 \right) + \sum_{\substack{w \sim v \\ w \neq u}} \binom{d(w)-1}{2} + (a-2) \left(\sum_{\substack{w \sim v \\ w \neq u}} d(w) - 1 \right) \end{aligned}$$

while for the $(0, 1)$ -cut:

$$\delta_S = \frac{3}{2} (d-1)(d-2)(d-3),$$

and

$$\delta_Y = \binom{a-1}{2} (d-1) + \binom{d-1}{2} (a-1) + \sum_{\substack{w \sim u \\ w \neq v}} \binom{d(w)-1}{2} + (d-2) \sum_{\substack{w \sim u \\ w \neq v}} (d(w) - 1),$$

and the same lower bound (as for the $(0,0)$ -cut) on δ_P holds.

We now consider three cases. Recall that by the choice of u and v we know that for $w \sim u, d(w) \leq \min\{a, d-1\}$ and for $w \sim v, d(w) \leq d$.

Case 1: $a = d$.

We use the $(0,0)$ -cut. It is enough to prove that

$$\begin{aligned} 3(d-1)(d-2)(d-3) &\geq 2 \binom{d-1}{2} (d-1) + \\ &\quad + \frac{1}{2}(d-1)^2(d-4) + \frac{1}{2}(d-1)(d-2)(d-5) + 6. \end{aligned}$$

This is equivalent to checking $d^2 - 6d + 9 \geq \frac{6}{d-1}$, which holds for $d \geq 5$.

Case 2: $a = d-1$.

We use the $(0,0)$ -cut. It is enough to prove that

$$\begin{aligned} &\frac{3}{2}(d-1)(d-2)(d-3) + \frac{3}{2}(d-2)(d-3)(d-4) \\ &\geq \binom{d-2}{2} (d-1) + \binom{d-1}{2} (d-2) + (d-1) \binom{d-2}{2} + \frac{1}{2}(d-2)(d-1)(d-6) + 6. \end{aligned}$$

This is equivalent to checking that $2d^2 - 15d + 31 \geq \frac{12}{d-2}$, which holds for $d \geq 5$.

Case 3: $a \leq d-2$.

We use the $(0,1)$ -cut. It is enough to prove that

$$\begin{aligned} &\frac{3}{2}(d-1)(d-2)(d-3) + (a-1) \sum_{\substack{w \sim u \\ w \neq v}} (d(w)-1) \\ &\geq \binom{a-1}{2} (d-1) + \binom{d-1}{2} (a-1) + \sum_{\substack{w \sim u \\ w \neq v}} \binom{d(w)-1}{2} + (d-2) \sum_{\substack{w \sim u \\ w \neq v}} (d(w)-1) + 6 \end{aligned}$$

Recall that for any $w \sim u, d(w) \leq a$, then it is enough to check

$$\begin{aligned} &\frac{3}{2}(d-1)(d-2)(d-3) \\ &\geq \binom{a-1}{2} (d-1) + \binom{d-1}{2} (a-1) + (d-1) \binom{a-1}{2} + (d-a-1)(d-1)(a-1) + 6 \\ &= \binom{d-1}{2} (a-1) + (d-3)(d-1)(a-1) + 6. \end{aligned}$$

The last term in the above display is maximized for $a = d-2$, and thus it is enough to check

$$\frac{3}{2}(d-1)(d-2)(d-3) \geq (d-3)(d-4)(d-1) + \binom{d-1}{2} (d-3) + (d-1)(d-3) + 6.$$

This inequality is equivalent to $1 \geq \frac{6}{(d-1)(d-3)}$ which holds for $d \geq 5$. ■

3 Some profiles outside the convex hull of simple millipedes

In this section we give a negative answer to the question posed in BL's open problem 1. Recall that we denote by $\mathcal{P}(k)$ the projection of $\Delta(k)$ onto the first two coordinates (those corresponding to paths and stars on k vertices).



Figure 1: A $(0, 0, 3, 4, 4, 3)$ -millipede.

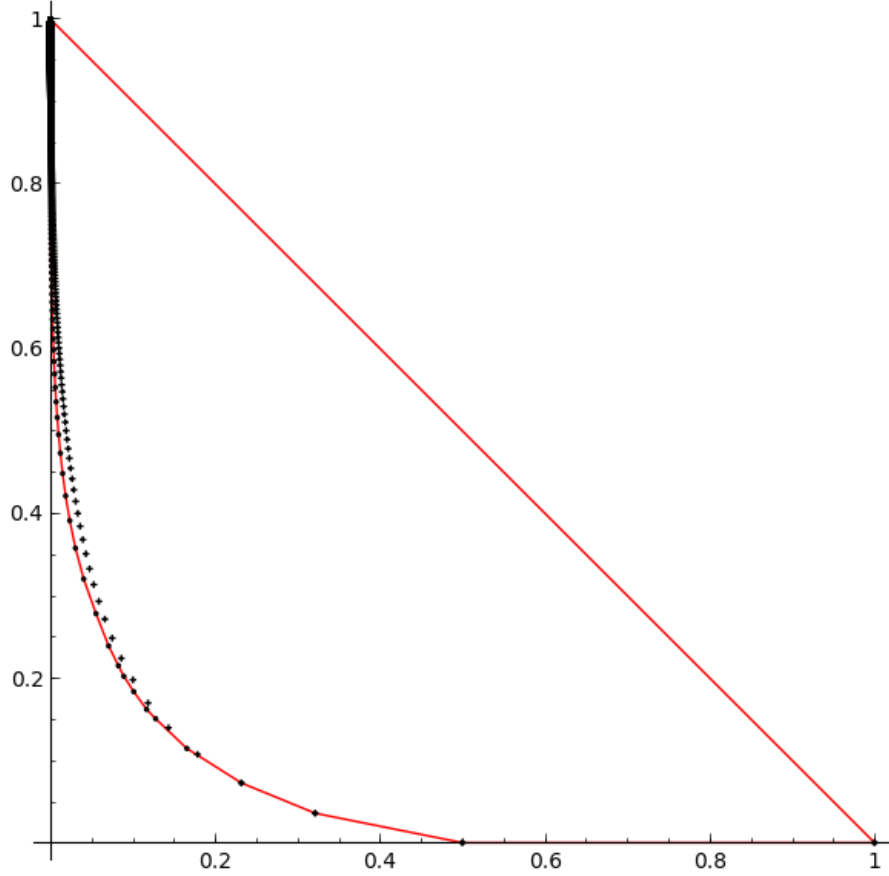


Figure 2: Points marked with '+' denote limiting profiles of (d) -millipedes. The red curve bounds the convex hull of a larger set of profiles.

Let $D = (d_1, \dots, d_\ell)$ be a finite sequence of integers. We say a graph T is a D -millipede if T consists of a path on vertices v_1, \dots, v_n , along with $d_i + 2$ pendant vertices at each vertex v_j with $j = i(\bmod \ell)$ (see Figure 1). We say that the D -millipede has length n . For a fixed sequence D , we write T_n^D to denote the D -millipede of length n .

BL asked whether all points in $\mathcal{P}(5)$ lie inside the convex hull of profiles of the sequences $(T_n^{(d)})$ of (d) -millipedes for $i \geq 0$. In fact $\mathcal{P}(5)$ contains the convex hull of the limiting 5-profiles corresponding to the following sequences of millipedes:

- (d) -millipedes; $0 \leq d \leq 3$
- $(0, 0, 3, 4, 4, 3)$ -millipede
- $(0, 0, d, d + 2, d + 2, d)$ -millipedes; $3 \leq d \leq 5$
- $(0, 0, d, d + 1, d)$ -millipedes; $4 \leq d \leq 6$
- $(0, 0, d, d)$ -millipedes; $d \geq 6$

This set strictly contains the limiting 5-profiles of (d) -millipedes. It is straightforward to compute the limiting profiles of the sequences (T_n^D) for each of the sequences describes above. We omit these tedious calculations and instead direct the reader's attention to Figure 2 for comparison.

In order to prove that the red curve in Figure 2 is tight, it would be sufficient to prove that each of an (infinite) sequence of linear inequalities holds for every tree. The first inequality is our Theorem 1, that $Y \leq 9S + P + 6$. The next few inequalities would be $Y \leq \frac{144}{29}S + \frac{42}{29}P + k_1$, then $Y \leq \frac{624}{175}S + \frac{66}{35}P + k_2$ and $Y \leq \frac{107}{40}S + \frac{5}{2}P + k_3$ (for universal constants k_i).

4 Few paths implies many stars

This section is dedicated to the proof of Theorem 2. This result offers a lower-bound on how fast the proportion of stars in a sequence of trees goes to one as the proportion of paths in the sequence goes to zero.

The key idea in the proof of Theorem 2 is to show that the number of non-star subtrees in a tree T is $\mathcal{O}(\sum d_i^\varepsilon)$ for some $\varepsilon < k - 1$, where $d_1, d_2, \dots, d_{|T|}$ is the degree sequence of T . If we can prove such a bound on the number of non-star k subtrees $R_k(T)$, the theorem follows because $S = \Omega(\sum d_i^{k-1})$. Why should one expect that there exists such a bound on $R_k(T)$? There are at most $(k-1)!D(T)^{k-1}$ subtrees with k nodes that contain a fixed vertex of maximum degree. Then an inductive argument yields an upper bound with $\varepsilon = k - 1$, but this bound is too weak for our purposes. If all the non-leaf nodes of T have the same degree, by the same method we obtain a bound with $\varepsilon = k - 2$ by removing one at a time nodes v with $d_v - 1$ neighboring leaves. The next proposition finds a middle ground.

Proposition 2 *Let T be a tree with degree sequence d_1, d_2, \dots, d_n . Then*

$$R_k(T) \leq e(k-1)! \sum_{d_i \geq 2} d_i^\varepsilon, \text{ where } \varepsilon = \frac{k-2 + \sqrt{(k-2)^2 + 4(k-2)}}{2}.$$

Proof

Label T 's nodes by v_1, v_2, \dots, v_n such that the first m are all the nodes with degree at least 2. Of course, d_i denotes the degree of node v_i . We employ the following strategy. We build the tree T from the empty set by adding some nodes at each step. Then we upper-bound the number of non-star trees added to the tree at each step and use these intermediate bounds to obtain the desired bound on $R_k(T)$.

The following construction of T meets our needs. Start with the tree T_1 : a star with $d_1 + 1$ nodes, centered at v_1 . Then, at each step, to construct T_{r+1} from T_r we choose a leaf node, which we label v_{r+1} , and attach to it $d_{r+1} - 1$ nodes in order to transform v_{r+1} into a node of degree d_{r+1} . Through appropriate choices of leaves at each step and maybe a relabeling of the nodes we can construct $T_m = T$.

Denote by S_r the set of non-star k -subtrees of T_r that contain at least one of the leaves added at step r . Hence, $R_k(T) = \sum_{r=2}^m |S_r|$ because $S_1 = \emptyset$. To upper-bound $|S_r|$ for all $r \geq 2$ we estimate the number of subtrees $S \in S_r$ based on the degrees of their nodes when viewed as nodes of T .

We denote by $U(S)$ the maximum degree of a non-leaf node of the k -subtree S when viewed as a node of T . We refer to the quantity $U(S)$ as the underlying degree of S in T . Now, for some $\alpha > 0$ to be chosen later, the sets S_r can be written as a disjoint union:

$$S_r = \{S \in S_r : U(S) \leq d_r^\alpha\} \sqcup \left(\bigsqcup_{u > d_r^\alpha} \{S \in S_r : U(S) = u\} \right).$$

First, we bound the number of subtrees in S_r with underlying degrees at most d_r^α . Since each such subtree is not a star, it contains the edge connecting v_r to T_{r-1} . Fix this edge and

call it e^* . We upper-bound the number of k -subtrees with underlying degree at most d_r^α that can be obtained by starting with e^* and adding new edges one at a time. Therefore, $k-2$ edges need to be added in order to obtain a k -subtree. If any of the endpoints of e^* has degree in T larger than d_r^α , then there are no $S \in S_r$ with $U(S) \leq d_r^\alpha$. On the other hand, if this is not the case, there are at most d_r^α choices for a new edge around each of the endpoints of e^* . So there are at most $2d_r^\alpha$ choices for the second edge of a subtree S . Once a choice is made so that the underlying degree remains at most d_r^α , there can be at most d_r^α new choices that can appear from adding a new edge. This means that after adding l edges, there are at most $(l+2)d_r^\alpha$ possible choices for a new edge. Hence, there are at most $\prod_{l=0}^{k-3} d_r^\alpha (l+2) = (k-1)! d_r^{\alpha(k-2)}$ subtrees in S_r with underlying degree at most d_r^α .

Now, each tree $S \in S_r$ with $U(S) > d_r^\alpha$ contains a node v_i , a non-leaf in S , with degree in T equal to $U(S)$, meaning $d_i = U(S)$. Observe that all the nodes on the path connecting v_i and v_r have degrees at most $U(S) = d_i$ in T by the definition of the underlying degree. Denote the distance between v_i and v_r with l_i , thus $1 \leq l_i \leq k-3$. By the same argument as in the one in the previous paragraph, there are at most $\frac{(k-1)!}{l_i!} d_r d_i^{k-2-l_i} \leq \frac{(k-1)!}{l_i!} d_i^{k-2-l_i+1/\alpha}$ such subtrees that contain both v_r and v_i . Then

$$|S_r| = \left| \bigcup_{u \geq 2} \{S \in S_r : U(S) = u\} \right| \leq (k-1)! d_r^{\alpha(k-2)} + (k-1)! \sum_{v_i} \frac{1}{l_i!} d_i^{k-2-l_i+\frac{1}{\alpha}},$$

where the sum is taken over all nodes v_i in T_{r-1} at distance at most $k-3$ from v_r with $d_i > d_r^\alpha$, and such that all the nodes on the path connecting v_i to v_r have degrees at most d_i . Summing over r gives an upper bound on $R_k(T)$.

For each $i \in [m]$ we upper bound the sum of all the terms containing a power of d_i that appear in the summation over r . It is easy to see that this sum is upper bounded by

$$(k-1)! d_i^{\alpha(k-2)} + (k-1)! \sum_{l=1}^{k-3} \frac{1}{l!} d_i^l d_i^{k-2-l+\frac{1}{\alpha}} \leq (k-1)! d_i^{\alpha(k-2)} + (e-1)(k-1)! d_i^{k-2+\frac{1}{\alpha}}$$

because in T there are at most d_i^l nodes at depth l away from v_i such that all the nodes on the path connecting them to v_i have degrees at most d_i (here e denotes Euler's constant). To obtain the conclusion we set $\alpha(k-2) = k-2 + \frac{1}{\alpha}$. ■

Remark that we found a bound on $R_k(T)$ with $k-2 < \varepsilon < k-1$. This bound is the main ingredient in the proof of the first part of Theorem 2.

Before we go into the proof of the theorem we reiterate the idea of gluing trees, used in [BL] to show that the set $\Delta_{\mathcal{T}}(k)$ is convex. Given two trees S and T we construct a new tree $S \boxtimes_k T$ by choosing a leaf in S and a leaf in T , and unite them with a path that contains $k-1$ newly added nodes. Hence the distance between the two chosen leafs in $S \boxtimes_k T$ is k . This construction depends on the choice of leafs, but this will not be an impediment for our future work.

Lemma 2 *Let S and T be two trees. Then for all $1 \leq i \leq N_k$*

$$c(T_i^k, S) + c(T_i^k, T) \leq c(T_i^k, S \boxtimes_k T) \leq c(T_i^k, S) + c(T_i^k, T) + (k-2)! D(S)^{k-3} + (k-2)! D(T)^{k-3}$$

$$Z_k(S) + Z_k(T) \leq Z(S \boxtimes_k T) \leq Z(T_i^k, S) + Z(T_i^k, T) + (k-2)! D(S)^{k-3} + (k-2)! D(T)^{k-3}.$$

Proof The left hand side inequalities are trivially true. We prove the upperbound on $Z_k(S \boxtimes_k T)$, the argument is based on similar ideas to the ones used in the proof of Proposition 2 and it will imply the other inequalities also.

We need to upperbound the number of k -subtrees that are formed by attaching a new vertex to a leaf node of S . It is clear that such a tree contains the new vertex, the leaf and the parent of the leaf. Hence, we need to count in how many ways $k-3$ nodes can be chosen from S to form a k -subtree. We do this iteratively. At the first step there are at most $D(S)$ choices and

after choosing each node, there can be at most $D(S)$ new choices. Then, at the second step there can be at most $2D(S)$ choices, at the third step $3D(S)$ and so forth. This means that there are at most $(k-3)!D(S)^{k-3}$ subtrees with k nodes that contain the new vertex. By the same procedure we see that there are at most

$$\sum_{i=0}^{k-3} (k-3-i)!D(S)^{k-3-i} + 1 \leq (k-2)!D(S)^{k-3}$$

k -subtrees formed by the $k-1$ vertices added by the gluing procedure together with S 's nodes. A similar bound holds for T and the upper bound for $Z_k(S \boxtimes_k T)$ follows. Remark that in this argument we upper-bounded the number of all k -subtrees that contain the new nodes, thus the other inequalities follow as well. \blacksquare

The next lemma will offer us a way to lower-bound the number of paths of the trees in a convergent sequence.

Lemma 3 *Let $(T_n)_{n \geq 1}$ be a sequence of trees such that $p^{(k)}(T_n) \rightarrow p$ and such that $D(T_n)$ is non-decreasing, and let*

$$T'_n = T_1 \boxtimes_k T_2 \boxtimes_k \dots \boxtimes_k T_n.$$

Then $p^{(k)}(T'_n) \rightarrow p$.

Proof

Since $Z_k(T_n) \rightarrow \infty$, by the Stolz-Cesàro theorem we know that

$$\lim_{n \rightarrow \infty} \frac{c(T_i^k, T'_n)}{Z_k(T'_n)} = \lim_{n \rightarrow \infty} \frac{c(T_i^k, T'_{n+1}) - c(T_i^k, T'_n)}{Z_k(T'_{n+1}) - Z_k(T'_n)},$$

if the right limit exists. By Lemma 2 we know that

$$\begin{aligned} \frac{c(T_i^k, T_{n+1})}{Z_k(T_{n+1}) + 2(k-2)!D(T_{n+1})^{k-3}} &\leq \frac{c(T_i^k, T'_{n+1}) - c(T_i^k, T'_n)}{Z_k(T'_{n+1}) - Z_k(T'_n)} \\ \frac{c(T_i^k, T'_{n+1}) - c(T_i^k, T'_n)}{Z_k(T'_{n+1}) - Z_k(T'_n)} &\leq \frac{c(T_i^k, T_{n+1}) + 2(k-2)!D(T_{n+1})^{k-3}}{Z_k(T_{n+1})} \end{aligned}$$

Remark that $Z_k(T_{n+1}) \geq \binom{D(T_{n+1})}{k-1}$ (look at the number of k -stars). Therefore the quotient $D(T_{n+1})^{k-3}/Z_k(T_{n+1}) \rightarrow 0$ as $n \rightarrow \infty$ and the conclusion follows. \blacksquare

Proof of the first part of theorem 2:

Let T_n be a sequence of trees with $|T_n| \rightarrow \infty$ whose sequence of profiles converges to p . Denote $|T_n| = v_n$ and let $d_{n,1}, d_{n,2}, \dots, d_{n,v_n}$ denote the degree sequence of T_n .

We can assume that $D(T_n)$ is non-decreasing by restricting to a subsequence. Then, Lemma 3 allows us to assume that $\text{diam}(T_n) \geq 2k$. It is not hard to check that in this case

$$P_k(T_n) \geq v_n - k.$$

Let $0 < \alpha < 1$ such that $\frac{\varepsilon}{1-\alpha} = k-1$. It is enough to prove that

$$\frac{R_k(T_n)}{Z_k(T_n) + k} \leq e(k-1)!(k-1)^\varepsilon \left(\frac{P_k(T_n) + k}{Z_k(T_n) + k} \right)^\alpha,$$

which is equivalent to proving

$$(R_k(T_n))^{\frac{1}{1-\alpha}} \leq (e(k-1)!)^{\frac{1}{1-\alpha}} (k-1)^{k-1} (P_k(T_n) + k)^{\frac{\alpha}{1-\alpha}} (Z_k(T_n) + k).$$

Proposition 2 and Jensen's inequality imply

$$\begin{aligned}
(R_k(T_n))^{\frac{1}{1-\alpha}} &\leq (e(k-1)!)^{\frac{1}{1-\alpha}} \left(\sum_{i=1}^{v_n} d_{n,i}^\varepsilon \right)^{\frac{1}{1-\alpha}} \leq (e(k-1)!)^{\frac{1}{1-\alpha}} (v_n)^{\frac{\alpha}{1-\alpha}} \sum_{i=1}^{v_n} d_{n,i}^{\frac{\varepsilon}{1-\alpha}} \\
&\leq (e(k-1)!)^{\frac{1}{1-\alpha}} (P_k(T_n) + k)^{\frac{\alpha}{1-\alpha}} \sum_{i=1}^{v_n} d_{n,i}^{k-1} \\
&\leq (e(k-1)!)^{\frac{1}{1-\alpha}} (P_k(T_n) + k)^{\frac{\alpha}{1-\alpha}} (k-1)^{k-1} (P_k(T_n) + k + S_k(T_n)) \\
&\leq (e(k-1)!)^{\frac{1}{1-\alpha}} (P_k(T_n) + k)^{\frac{\alpha}{1-\alpha}} (k-1)^{k-1} (Z_k(T_n) + k),
\end{aligned}$$

for the third inequality we used that $d^{k-1} \leq (k-1)^{k-1} \binom{d}{k-1}$ for all $d \geq k-1$. ■

In the case $k = 5$ we can improve this result by improving the upper-bound on $R_5(T)$.

Proposition 3 *Let T be a tree with degree sequence d_1, d_2, \dots, d_n . Then*

$$Y(T) \leq 2 \sum_{v=1}^n (d_v)^{2+\sqrt{3}}.$$

In addition, $2 + \sqrt{3}$ is the optimal exponent.

Proof Let us consider T 's orientation obtained by pointing all the edges away from vertex v_1 . Denote

$$A(v) = \{u \in V : (v, u) \in E \text{ and it points away from } v\}.$$

It is easy to check that

$$Y(T) = \sum_{v \in V} \sum_{u \in A(v)} \binom{d_u - 1}{2} (d_v - 1) + \binom{d_v - 1}{2} (d_u - 1).$$

Now, fix $v \in V$ and bound from above the sum

$$\sum_{u \in A(v)} \binom{d_u - 1}{2} (d_v - 1) + \binom{d_v - 1}{2} (d_u - 1) \leq \frac{1}{2} \sum_{u \in A(v)} (d_u)^2 d_v + (d_v)^2 d_u$$

We split the summation as follows. Let $A(v)^+ = \{u \in A(v) : d_v > (d_u)^\alpha\}$, where $\alpha > 1$ to be determined later, and let $A(v)^- = A(v) \setminus A(v)^+$. Also, let

$$\begin{aligned}
S_+ &= \frac{1}{2} \sum_{u \in A(v)^+} (d_u)^2 d_v + (d_v)^2 d_u \leq \frac{1}{2} \sum_{u \in A(v)^+} (d_v)^{\frac{2}{\alpha}+1} + (d_v)^{2+\frac{1}{\alpha}} \leq |A(v)^+| (d_v)^{2+\frac{1}{\alpha}} \leq (d_v)^{3+\frac{1}{\alpha}} \\
S_- &= \frac{1}{2} \sum_{u \in A(v)^-} (d_u)^2 d_v + (d_v)^2 d_u \leq \frac{1}{2} \sum_{u \in A(v)^-} (d_u)^{2+\alpha} + (d_u)^{1+2\alpha} \leq \sum_{u \in A(v)} (d_u)^{1+2\alpha},
\end{aligned}$$

where we used $|A(v)^+| \leq |A(v)| \leq d_v$ and $A(v)^- \subset A(v)$.

To obtain the best exponent to bound both S_+ and S_- we impose $3 + \frac{1}{\alpha} = 1 + 2\alpha$. Hence, $\alpha = \frac{1}{2}(1 + \sqrt{3})$. We obtain:

$$\sum_{u \in A(v)} \binom{d_u - 1}{2} (d_v - 1) + \binom{d_v - 1}{2} (d_u - 1) \leq S_+ + S_- \leq (d_v)^{2+\sqrt{3}} + \sum_{u \in A(v)} (d_u)^{2+\sqrt{3}}.$$

Summing over $v \in V$ yields the first part of the proposition.

Now, we prove the second part of the proposition. Consider a tree T of depth 2, rooted at a node r . Suppose the degree of r is d and each of r 's children has degree k . Then, it is immediate that

$$Y(T) = d \left(\binom{d-1}{2} (k-1) + \binom{k-1}{2} (d-1) \right)$$

Suppose $k = \lfloor d^\alpha \rfloor$ for some $\alpha > 0$ and suppose there exist $C, \varepsilon > 0$ such that:

$$Y(T) \leq C \sum_{v \in v} (d_v)^\varepsilon = Cd^\varepsilon + Cdk^\varepsilon + Cdk \leq Cd^\varepsilon + Cd^{1+\varepsilon\alpha} + Cd^{1+\alpha}.$$

Then, by letting d tend to infinity we see that all the following inequalities must hold $3 + \alpha \leq \max \{\varepsilon, 1 + \varepsilon\alpha, 1 + \alpha\}$, and $2\alpha + 2 \leq \max \{\varepsilon, 1 + \varepsilon\alpha, 1 + \alpha\}$. In other words, there must be no α that violates these inequalities. Suppose the first one is violated. Then, $\alpha > \varepsilon - 3$ and $\alpha < \frac{2}{\varepsilon-1}$. So if we want to be no α with these properties we need $\varepsilon - 3 = \frac{2}{\varepsilon-1}$, which yields $\varepsilon = 2 + \sqrt{3}$. ■

Proof of the second part of theorem 2: The argument is analogous to the one used in the proof of the first part of the theorem, but uses the stronger bound on $R_5(T)$ given by Proposition 3. ■

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